

Dantrolene
7261-97-4 | DTXSID7022881

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: 2.18

Global applicability domain: Inside

Local applicability domain index: 4.40e-01

Confidence level: 7.42e-01

Nearest Neighbors from the Training Set

Image not found

Dantrolene

Measured: 1.70

Predicted: 2.18

Image not found

2,6-Dinitro-4-(trifluoromethyl)aniline

Measured: 2.29

Predicted: 1.90